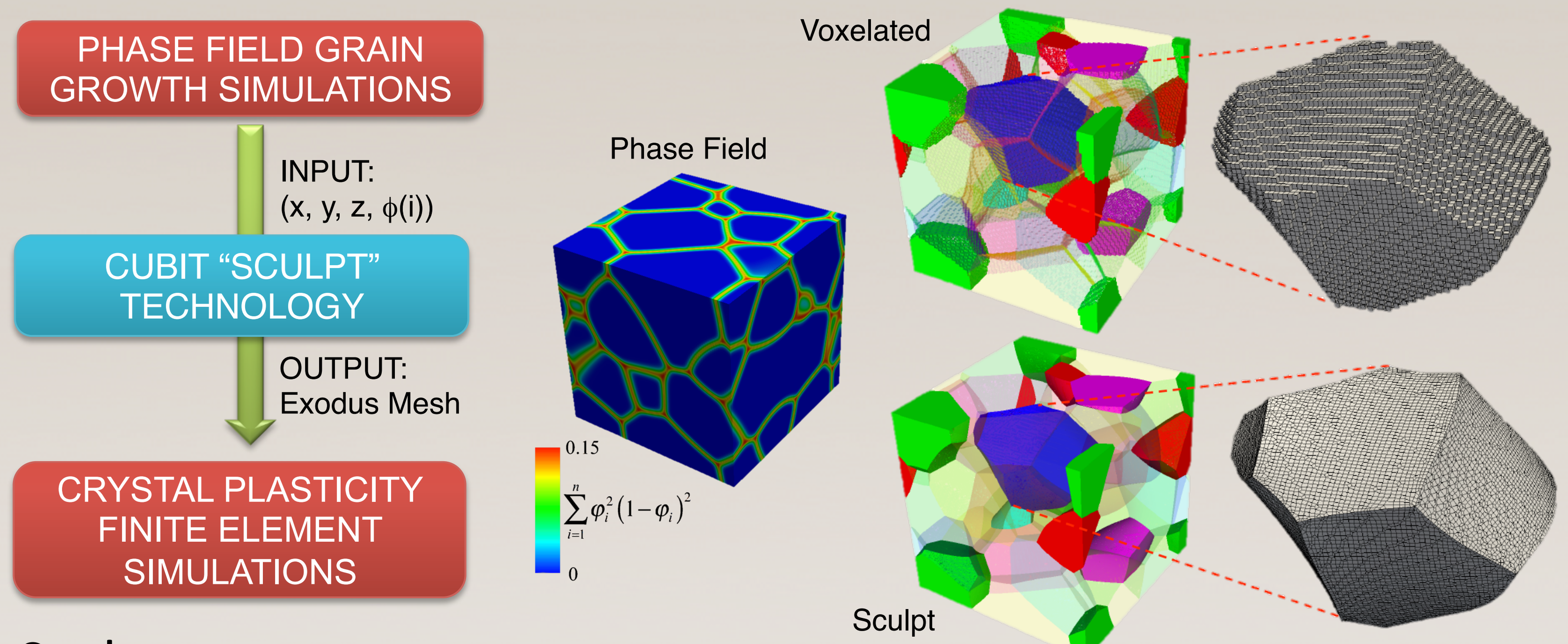
Hex Meshing for Microstructures

Exceptional service in the national interest

Steven Owen, Hojun Lim

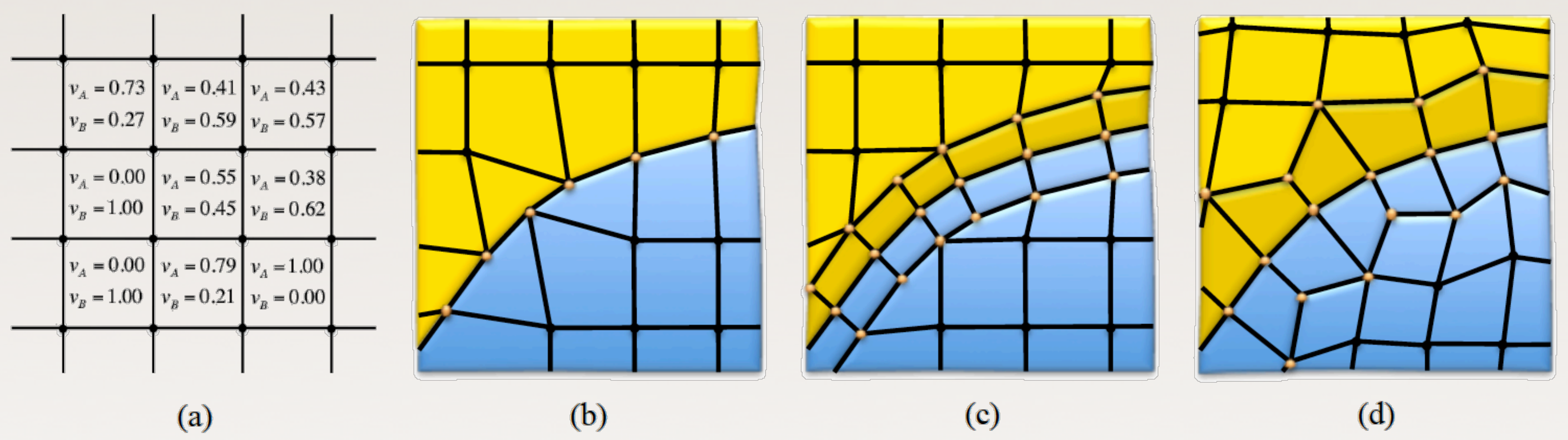
Sandia National Laboratories

Current technology for simulating mechanical responses of polycrystalline materials uses voxelated representations of microstructure. The objective of this study was to develop a tool for generating interface conforming all-hex FEA meshes of microstructures. Sandia's Sculpt tool was used as the basis for this study. Comparison of simulation results between voxelated and conforming FEA meshes was then performed using a crystal plasticity finite element model.



Sculpt

The Sculpt tool will generate an all hex mesh from volume fraction data on a Cartesian grid. Phase field data for microstructures in this case is a simple text file containing volume fractions for each grain or material per cell. Sculpt was modified to generate an all-hex mesh directly from phase field data.



(a) Initial volume fraction data on a Cartesian grid

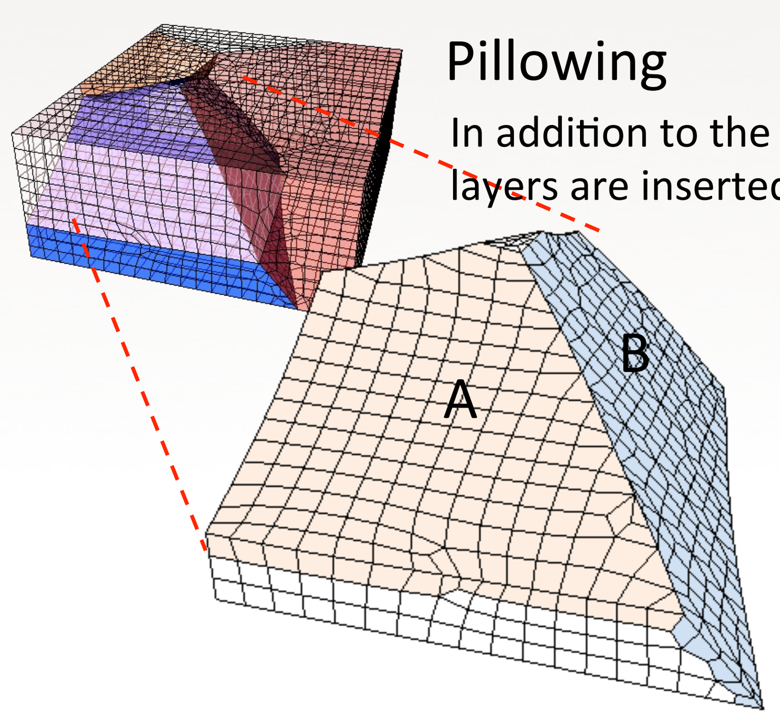
(b) Material interfaces reconstructed and grid nodes moved

(c) Layers of hexes inserted at interfaces

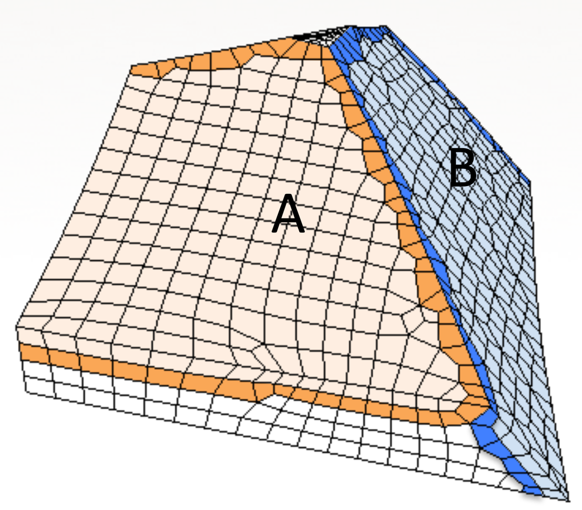
(d) Smoothing performed

Pillowing

In addition to the standard procedure outlined above, additional layers are inserted surrounding each unique interface surface.



Poor quality will result at Curve interfaces. Note triangle-shaped quads at curve between surfaces A and B



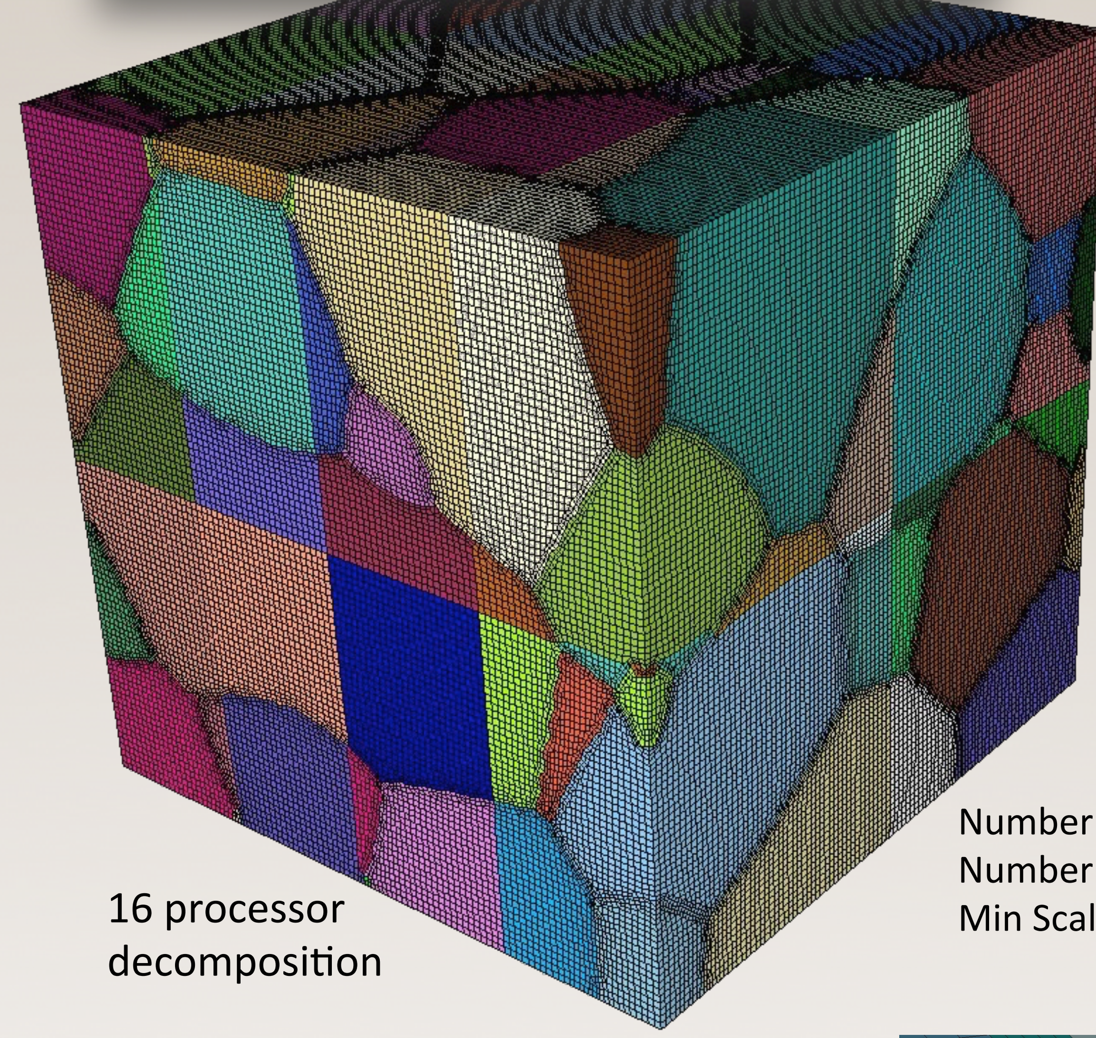
After pillows are inserted (darker elements), mesh quality is improved around curves.

Phase Field Data

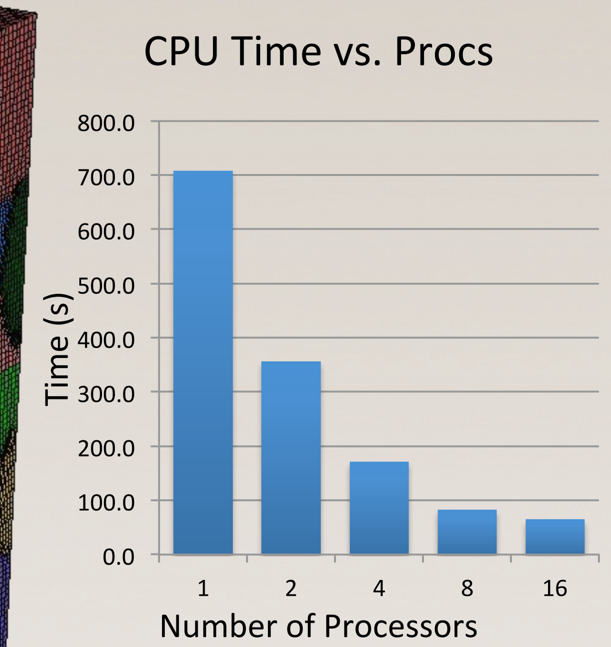
Example file format

```
TITLE = triple line system
VARIABLES = x y z, phi_1, phi_2, phi_3
ZONE i = 2 , j = 2 , k = 2
0.0000    0.0000    0.0000    0.5000    0.5000    0.0000
1.0000    0.0000    0.0000    0.3333    0.3333    0.3334
0.0000    1.0000    0.0000    1.0000    0.0000    0.0000
1.0000    1.0000    0.0000    0.0000    1.0000    0.0000
0.0000    0.0000    1.0000    0.2000    0.4000    0.4000
1.0000    0.0000    1.0000    0.6000    0.1000    0.3000
0.0000    1.0000    1.0000    0.0000    0.0000    1.0000
1.0000    1.0000    1.0000    0.9000    0.0000    0.1000
```

Data in text file is distributed amongst multiple processors. Each processor meshes its part of the global domain independently, maintaining continuity with MPI communication.



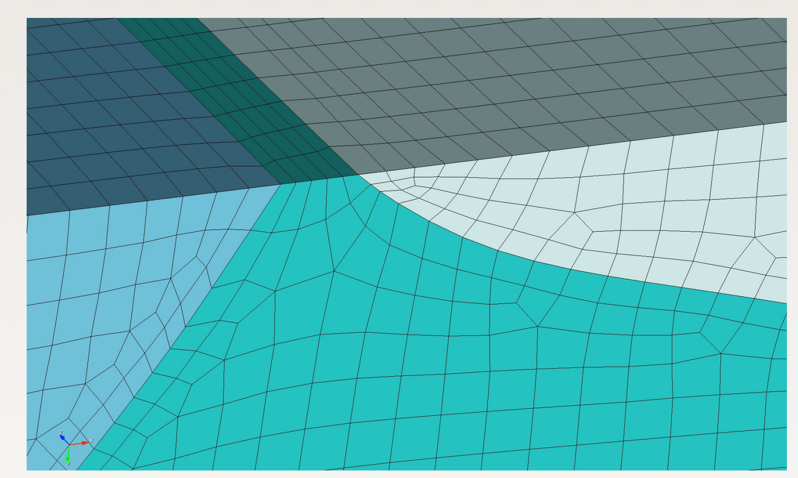
16 processor decomposition



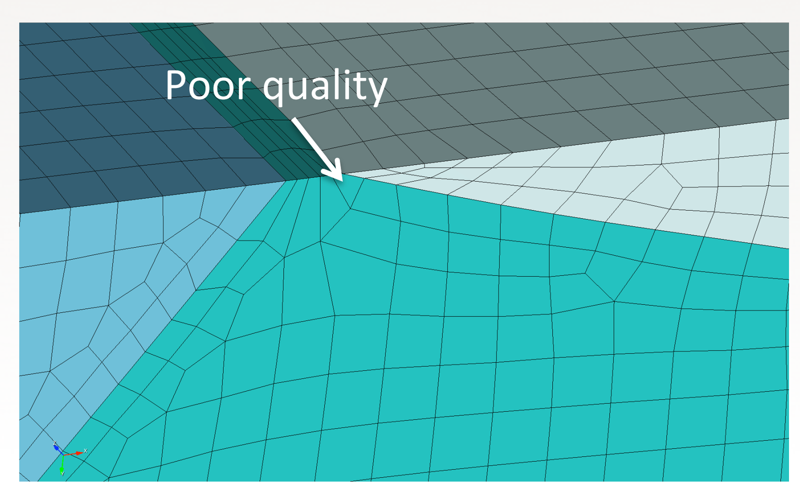
Number of Materials: 20
Number of Hexes: 1.35M
Min Scaled Jacobian: 0.209

Expansion Layers

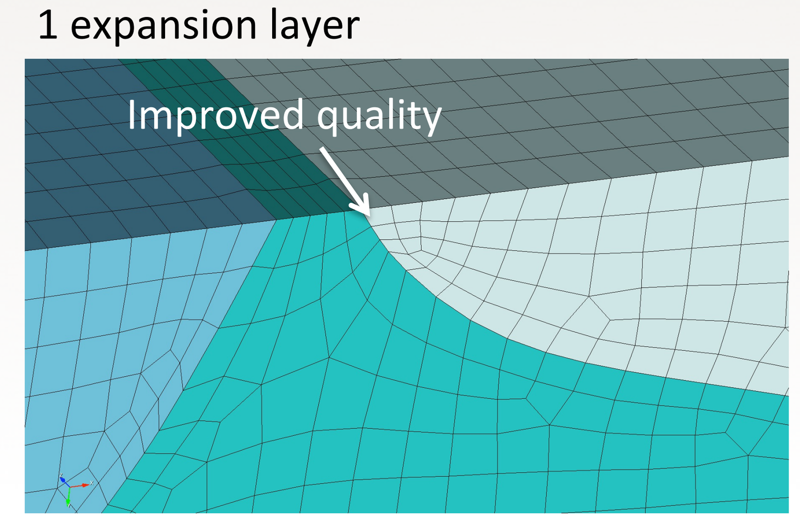
Where material interfaces intersect the boundary at small angles, The geometry can limit the quality of the mesh. One or more layers of cells can be added to the boundary of the Cartesian domain. The result is elements with improved quality.



1 expansion layer



No expansion.



2 expansion layers

Comparison of Simulation Results

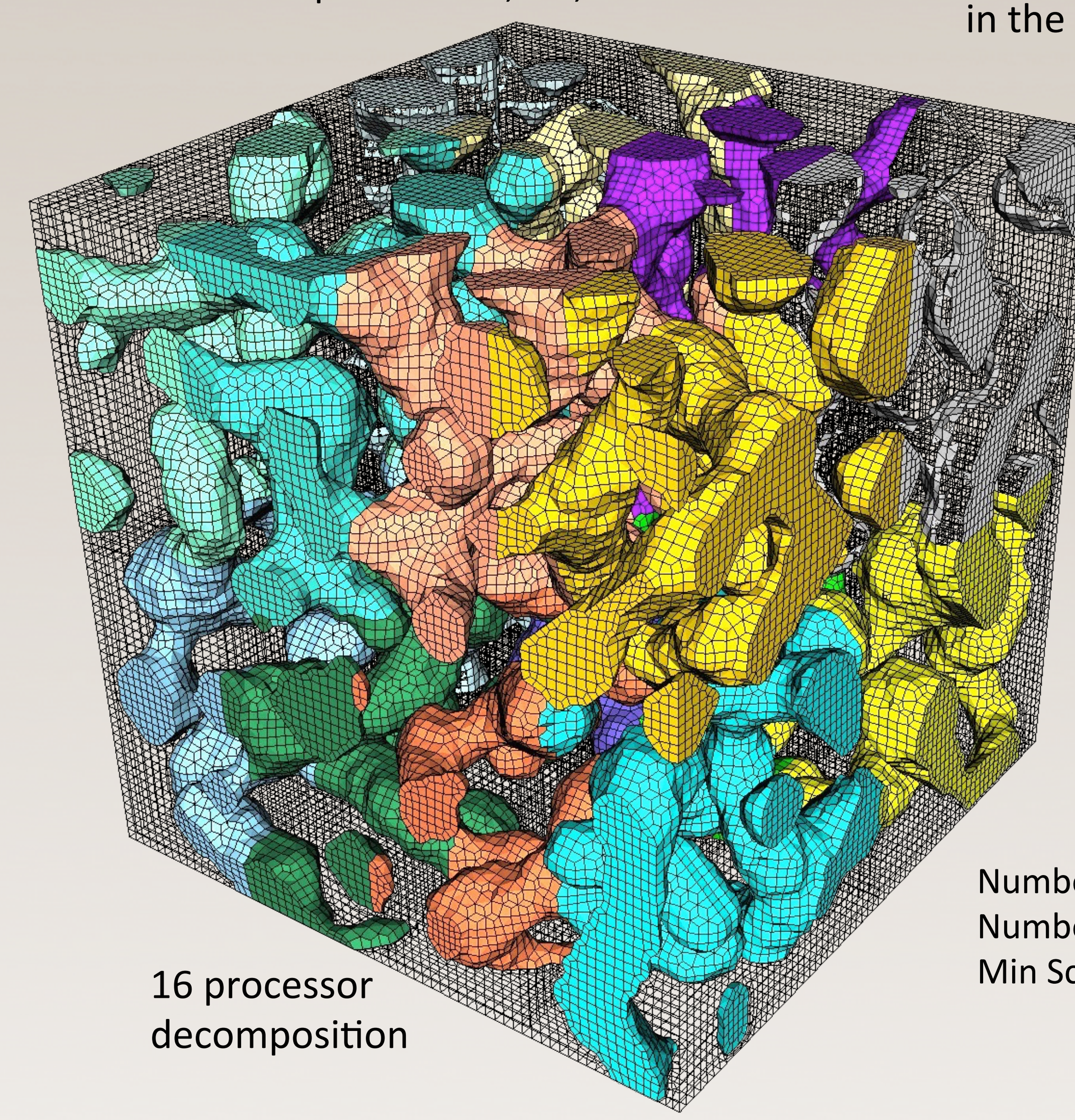
Initial results have shown that conformal interfaces provided by Sculpt will reduce artificial stress localizations observed in the voxelated mesh. Scaling of Sculpt's internal data structures will also be required to facilitate more realistic engineering-scale simulations of polycrystalline metals for a variety of mission-critical applications.

Two-Phase Monte Carlo Potts Simulations

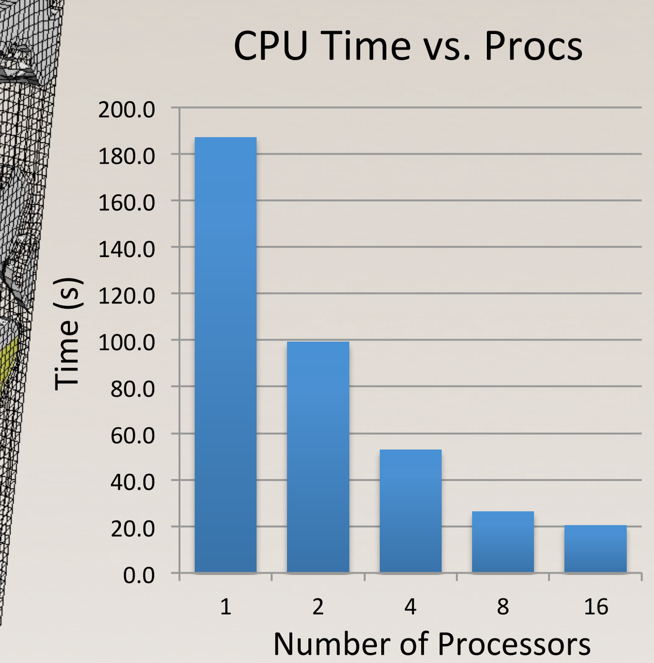
File Format

- Text file with 1 integer per cell
- Integer represents unique material ID
- User specifies NX, NY, NZ

A stair-step representation is converted to a smooth conformal mesh. In this case, volume fractions are either 0.0 or 1.0 for each material in the Cartesian grid.

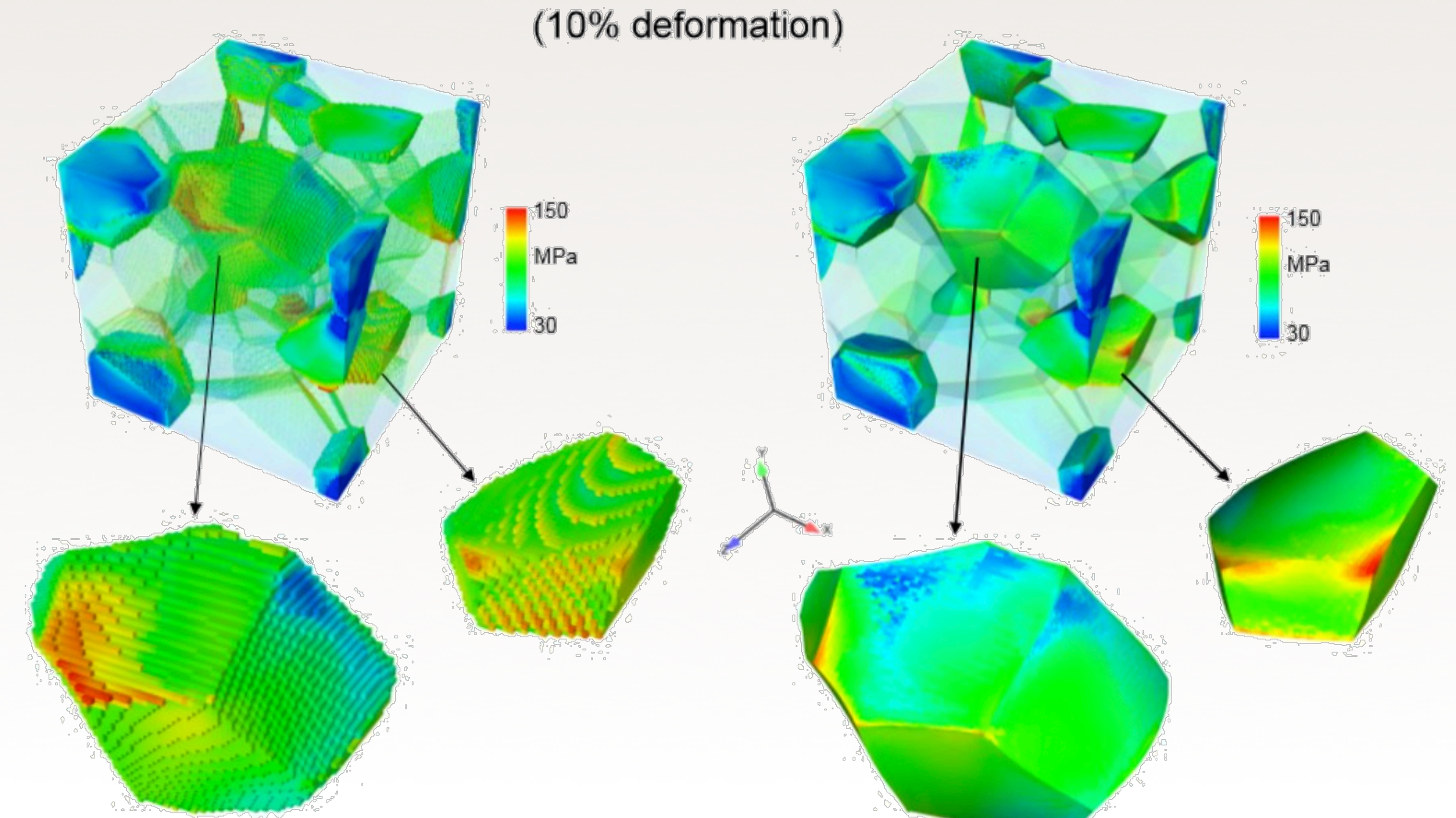


16 processor decomposition



Number of Materials: 2
Number of Hexes: 403K
Min Scaled Jacobian: 0.246

VonMises stress distributions (10% deformation)



Voxelated mesh

Conformal mesh

Impact

This effort delivers a practical computational capability based on materials science needs and leverages many ongoing works that involve large-scale finite element polycrystalline simulations. Further extension of this work will enable fundamental materials design and synthesis of application-optimized microstructures.

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.
SAND2015-8434 C